Effective hamiltonian approach for strongly correlated lattice models

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We review a recent approach for the simulation of many-body interacting systems based on an efficient generalization of the Lanczos method for Quantum Monte Carlo simulations. This technique allows to perform systematic corrections to a given variational wavefunction, that allow to estimate exact energies and correlation functions, whenever the starting variational wavefunction is a qualitatively correct description of the ground state. The stability of the variational wavefunction against possible phases , not described at the variational level can be tested by using the "effective Hamiltonian" approach. In fact Monte Carlo methods, such as the "fixed node approximation" and the present "generalized Lanczos technique" (Phys. Rev. B 64,024512, 2001) allow to obtain exact ground state properties of an effective Hamiltonian, chosen to be as close as possible to the exact Hamiltonian, thus yielding the most reasonable estimates of correlation functions. We also describe a simplified one-parameter scheme that improve substantially the efficiency of the generalized Lanczos method. This is tested on the $t - J$ model, with a special effort to obtain accurate pairing correlations, and provide a possible non-phonon mechanism for High temperature superconductivity.

1 Introduction

Despite the tremendous progress of computer performances the general task of determining the ground state wavefunction of a many-electron system is still far from being settled For instance, even for simplified models on a lattice, there is no general consensus on the ground state properties of a system of about 100 electrons on L 100 sites. The most striking example is the so called $t - J$ model: This model is still a subject of intense numerical studies, due to its possible relevance for High Tc superconductivity[1,2]. The Hamiltonian reads:

$$\hat{H} = J \sum_{\langle i,j \rangle} \left(\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j - \frac{1}{4} \hat{n}_i \hat{n}_j \right) - t \sum_{\langle i,j \rangle, \sigma} \tilde{c}_{i,\sigma}^\dagger \tilde{c}_{j,\sigma}, \tag{1}$$

where $\tilde{c}_{i,\sigma}^\dagger = \hat{c}_{i,\sigma}^\dagger (1 - \hat{n}_{i,\bar{\sigma}})$, $\hat{n}_i = \sum_\sigma \hat{n}_{i,\sigma}$ is the electron density on site i, $\hat{\mathbf{S}}_i = \sum_{\sigma,\sigma'} \tilde{c}_{i,\sigma}^\dagger \tau_{\sigma,\sigma'} \tilde{c}_{i,\sigma'}$ is the spin operator and $\tau_{\sigma,\sigma'}$ are Pauli matrices. In the following we consider N electrons on L sites, with periodic boundary conditions,(PBC), in order to minimize size effects.

After many years of intense numerical and theoretical efforts there is no general consensus on the properties of this simple Hamiltonian and of the related Hubbard model. In particular according to density matrix renormalization group (DMRG) studies [4], d-wave superconductivity is not stable in this model, whereas a ground state non uniform in density (with so called "stripes") is found. Several QMC studies provide controversial results, most of them indicating a superconducting behavior, and some of them[5], indicating the opposite.

The reason of the above controversy, can be easily explained within the straightforward variational approach. Whenever a model Hamiltonian cannot be solved exactly either numerically (with no sign problem) or analytically, the most general and reasonable approach is an approximate minimization of the energy within a particular class of wavefunctions, for instance also DMRG can be considered a variational approach with a particularly complicated variational wavefunction obtained by DMRG iterations. However, within the variational approach, one faces the following problem: for large system size L the gap to the first excited state scales generally to zero quite rapidly with L. Thus between the ground state energy and the variational energy there maybe a very large number of states with completely different correlation functions. In this way one can generally obtain different variational wavefunctions with almost similar energy per site, but with completely different correlation functions. It is easily understood that, within a straightforward variational technique, there is no hope to obtain sensible results for large system size, unless for for system with a finite gap to all excitations, such as spin liquid[6], or band insulators..

In the following we are trying to argue that a possible solution to the previous limitation of the variational technique is provided by what we call in the following "the effective Hamiltonian approach".

This approach relies on the following assumption:

"Among similar Hamiltonians with local interactions the ground state correlation functions depend weakly on the details of the Hamiltonian, in a sense that similar Hamiltonians should provide similar correlation functions"'. In this way the ground state of an effective Hamiltonian (such as the fixed node Hamiltonian[8]) that can be solved exactly by Quantum Monte Carlo schemes can be used as a variational state of the desired Hamiltonian, in this way providing not only a good variational energy but the most reasonable estimate of correlation functions, as long as the variational energy obtained is close -but not terribly close as in the straightforward variational approach- to the exact ground state energy.

The paper is based therefore on the recent numerical advances for solving approximately model Hamiltonians on a lattice: the fixed node[8], and the "generalized Lanczos technique"[3], that allows to improve systematically the variational energy provided by the effective Hamiltonian approach, by combining in an efficient way the power of the Lanczos variational technique with the "effective Hamiltonian approach". Trough all the paper and pictures we will use "FN" to indicate the "fixed node approach", , whereas "SR "will indicate the . "stochastic reconfiguration method" used to apply the "generalized Lanczos" scheme. In the first part we describe the Lanczos technique, then we derive the effective Hamiltonian approach in a slightly more general way than the standard "fixed node" method. Finally we show that the mentioned "generalized Lanczos method" represents a very efficient implementation of both the previous techniques- Lanczos and fixed node- on a lattice. We also point out some slight but important improvements and simplifications to the most recent formulation of the "generalized Lanczos scheme"[3]. In the last section before the conclusion we show some example on the t-J model, where the "effective Hamiltonian approach" is clearly useful, as the pairing correlation functions appear to be rather independent from the initial variational guess, even for large system size $L \simeq 50$ and small J/t.

2 The Lanczos technique

The Lanczos technique represents a remarkable improvement of the power method used to filter out systematically the ground state component of a given initial wavefunction ψ_G by an iterative technique. The power method is based on the following equation:

$$\psi_0\rangle \simeq (\Lambda I - H)^p |\psi_G\rangle \tag{2}$$

where Λ is a suitable large shift to ensure convergence to the ground state for large p, I is the identity matrix and $|\psi_0\rangle$ the ground state of H. At a given iteration p, after applying just p powers of the Hamiltonian, a much better wavefunction ψ_p can be obtained by combining, with proper coefficients α_k, the states obtained with the power method in the previous iterations:

$$|\psi_p\rangle = \Big(1 + \sum_{k=1}^{p} \alpha_k H^k\Big)|\psi_G\rangle \tag{3}$$

with parameters $\{\alpha_k\}$ for $k = 1, \cdots, p$ minimizing the energy expectation value $\langle\psi_p|\hat{H}|\psi_p\rangle/\langle\psi_p|\psi_p\rangle$. For any p it is simple to show that the wavefunction (3) corresponds exactly to apply p Lanczos step iterations to the initial wavefunction $|\psi_G\rangle$. The $H-$polynomial of degree p which is applied to the initial state ψ_G, can be generally factorized in terms of its roots z_i:

$$\Big(1 + \sum_{k=1}^{p} \alpha_k \hat{H}^k\Big) = \prod_{i=1}^{p}(1 - H/z_i) \tag{4}$$

This decomposition will be particular important for applying statistically the Lanczos technique with the Stochastic Reconfiguration (see later). As it is clear from Fig. (1), the Lanczos method converges very quickly to the ground state wavefunction especially when a particularly good "guess" is used for ψ_G.

Whenever the ground state wavefunction is approached $|\langle\psi_0|\psi_p\rangle|^2/\langle\psi_p|\psi_p\rangle^2 = 1-\epsilon_p$, with $\epsilon_p \to 0$ for larger p, with the energy approaching the exact value with corrections $\simeq \epsilon_p$. On the other hand, the variance σ_p^2 of the Hamiltonian on the approximate state ψ_p

$$\sigma_p^2 = \langle\psi_p|H^2|\psi_p\rangle - \langle\psi_p|H|\psi_p\rangle^2 = O(\epsilon_p)$$

is going to zero in the limit when ψ_p is the exact eigenstate ψ_0 with the same corrections proportional to ϵ_p.: It is clear therefore that a very stable evaluation of the energy can be done by using few Lanczos steps values of the energy and the corresponding variance. Then, by performing simple extrapolation (linear or even polynomial), the exact ground state result is easily estimated provided the energy-variance values are close to the linear regime (see Fig.1). The same scheme can be applied even for correlation functions[3], and represents one of the most simple and effective methods to estimate exact correlation functions with few Lanczos steps (i.e. with a minor computational effort) whenever the variational wavefunction ψ_G is particularly good, i.e. is close to the linear energy vs. variance regime. Such property of the variational wavefunction can be satisfied even for system size $L \simeq 100^3$.

The initial wavefunction to which the Lanczos and the following techniques will be applied can be written as follows [10]:

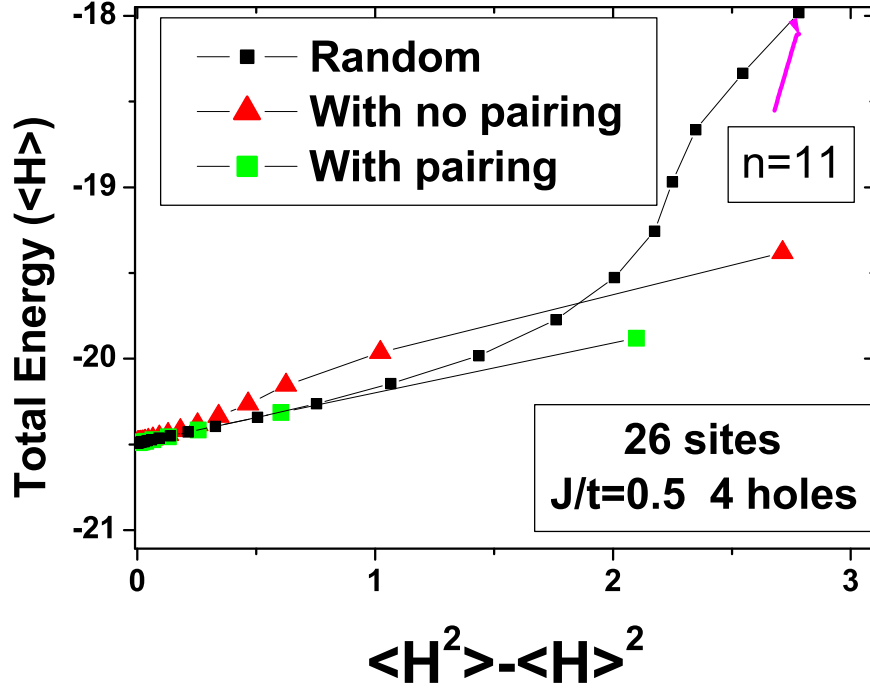$$|\psi_G\rangle = |\psi_{p=0}\rangle = \hat{P}_0\,\hat{P}_N\hat{J}|D\rangle. \tag{5}$$

Figure 1. Energy $<H>$ vs. variance $<H^2> - <H>^2$ of the Lanczos technique for different initial wavefunction ψ_G. Here n represents the number of iterations. Lower variance is always obtained for larger n. The zero variance limit is the exact results.

where $|D\rangle$ is a BCS wavefunction, which is an exact eigenstate of the following Hamiltonian:

$$\hat{H}_{BCS} = \hat{H}_0 + \frac{\Delta_{BCS}}{2}(\hat{\Delta}^\dagger + \hat{\Delta}) \qquad (6)$$

$$\hat{\Delta}^\dagger = \sum_{\langle i,j \rangle} M_{i,j}\left(\tilde{c}^\dagger_{i,\uparrow}\tilde{c}^\dagger_{j,\downarrow} + \tilde{c}^\dagger_{j,\uparrow}\tilde{c}^\dagger_{i,\downarrow}\right) \qquad (7)$$

where $\hat{H}_0 = \sum_{k,\sigma} \epsilon_k \tilde{c}^\dagger_{k,\sigma}\tilde{c}_{k,\sigma}$ is the free electron tight binding nearest-neighbor Hamiltonian, $\epsilon_k = -2(\cos k_x + \cos k_y) - \mu$, μ is the free-electron chemical potential and $\hat{\Delta}^\dagger$ creates all possible singlet bonds with d-wave symmetry being $M_{i,j}$, $M_{i,j}$ not restricted to nearest neighbors, but exhaustively parametrized with a reasonable number of variational parameters as described in [3]. $\hat{P}_N$ and $\hat{P}_0$ are the projectors over the subspaces with a fixed number N of particles and no doubly occupied states. Finally the Jastrow factor $\hat{J} = \exp\left(1/2 \sum_{i,j} v(i-j)\hat{n}_i\hat{n}_j\right)$ couples the holes via the density operators $\hat{n}_i$ and con-

tains other few variational parameters. We note here that by performing a particle-hole transformation on the spin down $\tilde{c}_{i,\downarrow}^{\dagger} \rightarrow (-1)^i \tilde{c}_{i,\downarrow}$, the ground state of the BCS Hamiltonian is just a Slater-determinant with $N = L$ particles [11]. This is the reason why this variational wavefunction can be considered of the generic Jastrow-Slater form, a standard variational wavefunction used in QMC. All the mentioned variational parameters are obtained by minimizing the energy expectation value of H over ψ_G[3].

Using the particle-hole transformation, it is also possible to control exactly the spurious finite system divergences related to the nodes of the d-wave order parameter.

3 The effective Hamiltonian approach

In a discrete Hilbert space defined for instance by configurations x of electrons with definite positions and spins we consider *any* Hamiltonian H with real matrix elements $H_{x',x}$ and *any* real wavefunction $\psi_G(x)$ assumed to be non zero for each configuration x.

By means of the wavefunction ψ_G-hereafter called the guiding wavefunction- we can define a two parameter class of Hamiltonians H_{FN}^{γ} depending on γ and r:

$$
H_{FN}^{\gamma} = \begin{cases} H_{x,x} + (1+\gamma)\mathcal{V}_{sf}(x) + r(1+\gamma)e_L(x) & \text{for } x' = x \\ H_{x',x} & \text{if } x' \neq x \quad \text{and } \psi_G(x')H_{x',x}/\psi_G(x) < 0 \\ -\gamma H_{x',x} & \text{if } x' \neq x \quad \text{and } \psi_G(x')H_{x',x}/\psi_G(x) > 0 \end{cases}
$$

(8)

where the local energy $e_L(x)$ is defined by:

$$
e_L(x) = \sum_{x'} \psi_G(x')H_{x',x}/\psi_G(x)
$$

(9)

and the so called sign-flip term $\mathcal{V}_{sf}(x)$ introduced in [8] is given by considering the sum of all the *positive* off-diagonal matrix elements appearing in the local energy. The effective Hamiltonian H^{γ} has the *same* matrix elements of the Hamiltonian H for all off-diagonal matrix elements that do not frustrate the guiding function signs, the other ones are taken into account by proper modification of the diagonal term.

The following properties are almost an immediate consequence of the above definitions:

i) for $\gamma = -1$ $\qquad H = H_{FN}^{\gamma}, .$
ii) for $r = -1/(1+\gamma)$ and $\gamma \neq -1$ the ground state of H_{FN}^{γ} is the guiding wavefunction itself with zero ground state energy, namely $H_{FN}^{\gamma}|\psi_G\rangle = 0$.
iii) $H = H_{FN}^{\gamma} - (1+\gamma)\frac{dH_{FN}^{\gamma}}{d\gamma}$
iv) $E_L(x) = \sum_{x'} \psi_G(x')H_{FN}^{\gamma}/\psi_G(x) = e_L(x)(1 + r(1+\gamma))$ where $E_L(x)$ is the local energy of the effective Hamiltonian H_{FN}^{γ}, whereas $e_L(x) = \sum_{x'} \psi_G(x')H/\psi_G(x)$. the corresponding one for H. Moreover:
(v) for $\gamma \geq 0$ the ground state $\psi_0^{FN}(x)$ of H_{FN}^{γ} may be chosen to have the same signs of the guiding wavefunction, namely $\psi_G(x)\psi_{FN}(x) \geq 0$ for any configuration x. This follows by doing a unitary transformation of the basis $|\bar{x}\rangle = \text{Sign}[\psi_G(x)]|x\rangle$, in which the off-diagonal matrix elements of the Hamiltonian $H_{FN,\bar{x}',\bar{x}}^{\gamma} < 0$ are non-positive. Thus

the Perron-Frobenius theorem holds implying that a ground state wavefunction (in principle there maybe degeneracy) can be chosen to satisfy $\psi_0^{FN}(\bar{x}) \geq 0$ in the new basis, which finally proves (v) in the original basis. The statement (v) suggests that the effective Hamiltonian H_{FN}^γ represents the lattice counterpart of the fixed node (FN) hamiltonian, a well known approximation for continuous models.[9] Furthermore, provided the matrix elements of the hamiltonian H or H^{FN} satisfy an ergodicity property (namely that any two arbitrary configurations x and x' can be always connected by a suitable large number M of hamiltonian powers $\langle x'|H^M|x \rangle \neq 0$), then a more restrictive property holds: the ground state is unique for any $\gamma \geq 0$. This implies immediately that:

(vi) the ground state energy $E(\gamma)$ of the fixed node hamiltonian H_{FN}^γ is an analytic function of γ, due to the finite size gap separating the unique ground state from the first excited state. We assume in the following that this very general property holds for the given hamiltonian a condition which is not restrictive, also considering that if ergodicity is not satisfied, all previous and the following considerations hold in all the subspaces of configurations x ergodically connected by the powers of the hamiltonian.

By using Green Function Monte Carlo the ground state energy $E(\gamma)$ can be very efficiently computed for $\gamma > 0$ as all the matrix elements of the importance sampled Green function $G_{x',x}^{FN} = \psi_G(x')\left[\Lambda \delta_{x',x} - (H_{FN}^\gamma)_{x',x}\right]/\psi_G(x)$ are all positive for large enough constant shift Λ. This is obtained by averaging the local energy $< E_L(x) >$ over the configurations x generated statistically by the Green function G^{FN} with a standard algorithm.[7,12,13] Notice also that, by property (iv), the local energy E_L of this fixed node hamiltonian is proportional to the local energy e_L of H and therefore this computation satisfy the so called zero variance property: both E_L and e_L have zero statistical variance if ψ_G is an exact eigenstate of H.

For $r = 0$ H_{FN}^γ reduces to the standard fixed node hamiltonian defined in [8] ($\gamma = 0$) and extended to $\gamma \neq 0$ in [14]. Thus a rigorous theorem holds relating the ground state energy $E(\gamma)$ of the fixed node ground state ψ_{FN}^γ of H_{FN}^γ, to its variational expectation value $E^{FN}(\gamma) = \langle \psi_{FN}^\gamma|H|\psi_{FN}^\gamma \rangle$ on the hamiltonian H:

$$E^{FN}(\gamma) \leq E(\gamma) \leq \langle \psi_G|H|\psi_G \rangle \qquad (10)$$

Using property (i) we therefore notice that by increasing the value of r from the variational value $r = -1/(1 + \gamma)$ up to $r = 0$ the ground state of the fixed node hamiltonian H_{FN}^γ becomes a variational state with lower energy expectation value. This implies immediately that the fixed node effective hamiltonian is more appropriate to describe the ground state of H.

In the continuous case r cannot be extended to positive values because the local energy e_L may assume arbitrary large negative values close to the nodes, and the best variational energy can be actually obtained just for $r = 0$ (since for $r = 0$ the fixed node gives the lowest possible energy compatible with the nodes of the guiding function). In a lattice case such a theorem is missing, and there is no reason to expect that $r = 0$ is just the optimal value.

A simple and efficient scheme to compute a variational upper bound of the energy for

any r is described in the following paragraphs. Using property (iii)

$$E_{FN}(\gamma) = \langle\psi_{FN}^\gamma|H^\gamma - (1+\gamma)\frac{dH_{FN}^\gamma}{d\gamma}|\psi_{FN}^\gamma\rangle = E(\gamma) - (1+\gamma)\frac{dE(\gamma)}{d\gamma} \qquad (11)$$

where in the latter equality the Hellmann-Feynmann theorem has been used. By using that H_{FN}^γ depends linearly on γ, the well known convexity property of $E(\gamma)$ holds[15] :

$$\frac{d^2E(\gamma)}{d\gamma^2} \leq 0 \qquad (12)$$

Therefore the expectation value $E_{FN}(\gamma)$ of the hamiltonian H on the fixed node state is a monotonically increasing function of γ), as clearly $\frac{dE_{FN}(\gamma)}{d\gamma} = -(1+\gamma)\frac{d^2E(\gamma)}{d^2\gamma} \geq 0$. The best variational estimate is obtained therefore for $\gamma = 0$, as in the conventional scheme.

The extension to finite γ is however convenient to provide better variational estimates of $E_{FN}^{\gamma=0}$, which in fact maybe sizable lower than the standard estimate $E_{FN}(0) \leq E(0)$ for $r = 0$. This extension allows also to make a rigorous upper bound of E_{FN}^γ also in the case $r > 0$, without missing the zero variance property. In fact, always by the convexity property of $E(\gamma)$,

$$-\frac{dE(\gamma)}{d\gamma}|_{\gamma=0} \leq -\frac{E(\gamma) - E(0)}{\gamma} \qquad (13)$$

we finally get that at the best variational condition $\gamma = 0$

$$E_{FN}(0) \leq E(0) - (E(\gamma) - E(0))/\gamma. \qquad (14)$$

For $r = 0$ the above upper bound improves also the previously known value (10), at least for γ small enough where the above inequality becomes a strict equality.

In practice, since the energy as a function of γ is almost linear a very good estimate can be obtained using the above inequality even for $\gamma = 1$, as shown in Fig.(2) for a test example on the $t - J$ model, where it is also clear that the variational energy can be improved by turning on the parameter r.

4 The generalized Lanczos

The optimization of the parameter r is rather problematic within the scheme of the previous section especially when few Lanczos steps are applied to the guiding function and the dependence of the energy as a function of r cannot be resolved within available statistical errors. Though the energy maybe rather insensitive to r, the behavior of correlation functions, may strongly depend on it, especially when the guiding function shows some instability towards different phases not described at the variational level. Within this approach the instability of the guiding function is characterized by the existence of a considerable number of configurations x with local energy $e_L(x)$ much below the average and with correlation properties much different than the average. By increasing r these configurations will have larger and larger weight in the fixed node ground state ψ_{FN}^γ (since they have much lower-energy diagonal term) and will display clearly the possible instabilities of the variational wavefunction ψ_G.

The sign-flip term $\mathcal{V}_{sf}(x)$ is divergent whenever the guiding function is exceedingly small (i.e. close to the nodes or finite-size lattice pseudo-nodes of ψ_G), thus requiring
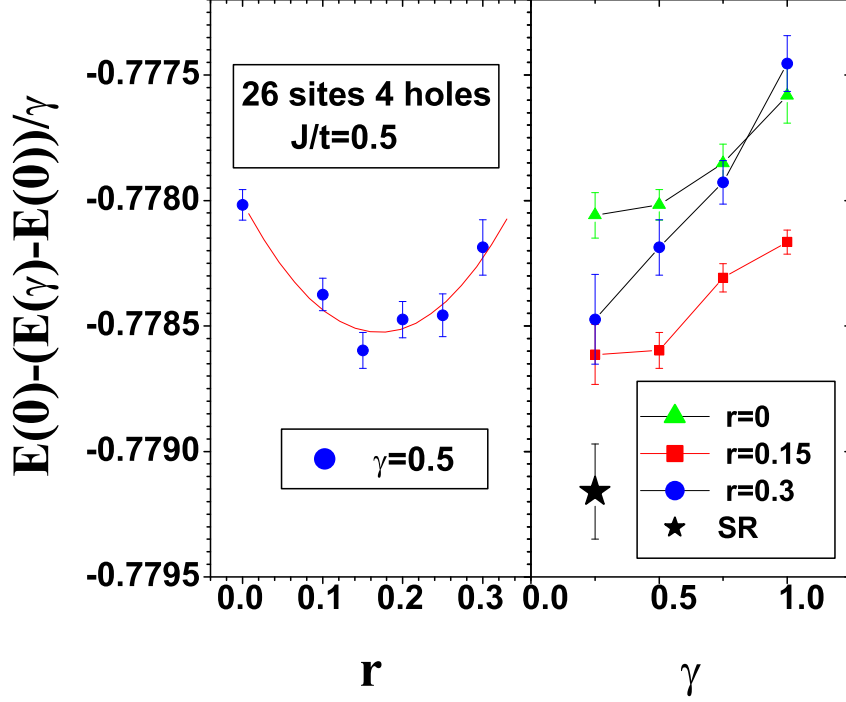
Figure 2. Variational energy of the t-J hamiltonian as a function of the parameters r and γ, for the BCS-guiding function (5), without any Lanczos improvement. The $\gamma \to 0$ limit in the right panel corresponds to the expectation value $E^{FN}(\gamma) = \langle \psi_{FN}^\gamma | H | \psi_{FN}^\gamma \rangle$ for $\gamma = 0$ where ψ_{FN}^γ is the ground state of the effective hamiltonian H_{FN}^γ. Each point, due to inequality (14), represents an upper bound for $E^{FN}(\gamma = 0)$ and, clearly, for the ground state of H. All the estimates reported here are much better than the standard $r = 0$ lattice fixed node upper bound $E(\gamma = 0)$[8] for $E^{FN}(\gamma = 0)$: $E(\gamma = 0) = -0.77580(2)$ much above the upper energy scale. The value (SR) obtained with the "generalized Lanczos" described in the following sections is also shown for comparison.

an infinite shift Λ[14], because for the statistical implementation of the power method the diagonal term $\Lambda - (H_{FN}^\gamma)_{x,x} = \Lambda - H_{x,x} - (1 + \gamma)\mathcal{V}_{sf}(x) - r(1 + \gamma)e_L(x)$ (see Eq.8) has to be non negative. For $r = -1/(1 + \gamma)$, in the variational case, a better approach, but similar in spirit, is obtained by sampling[16] the square of the variational wavefunction ψ_G with a different Green function. This following importance sampled Green function is used for the statistical implementation of the power method:

$$G_{x',x}^\gamma = \begin{cases} \frac{1}{z_{x'}}(\Lambda - H_{x,x}) & \text{for } x' = x \\ -\frac{1}{z_{x'}}\psi_G(x')(H_{FN}^\gamma)_{x',x}/\psi_G(x) & \text{for } x' \neq x \end{cases} \qquad (15)$$

where z_x is a normalization factor obtained by setting $\sum_{x'} z_{x'} G^{\gamma}_{x',x} = z_x$, namely:.

$$z_x = \Lambda - e_L(x) + (1 + \gamma)\mathcal{V}_{sf}(x) \tag{16}$$

In this way it is straightforward to show that:

$$\sum_x G^{\gamma}_{x',x} |\psi_G(x)|^2 = |\psi_G(x)|^2 \tag{17}$$

Thus the importance-sampled Green function G^{γ} maybe used to generate configurations that sample the variational wavefunction square. The advantage of the present approach is evident since the diagonal term of the Green function does not contain the sign-flip term, and a finite reasonable Λ can be used. For instance in the $t - J$ model Λ can be set to zero. Instead a zero shift is not allowed for the importance sampled Green function of the effective hamiltonian itself:

$$G_{FN} = \psi_G(x') \left[\Lambda - (H^{\gamma}_{FN})_{x',x} \right] / \psi_G(x) \tag{18}$$

which performs the same task for $r = -1/(1 + \gamma)$, but with a less efficient infinite Λ scheme[14].

In the following, within the spirit of the "effective hamiltonian approach", the variational wavefunction is improved by tuning a parameter r proportional to the local energy, in order to modify and improve the effective hamiltonian H^{γ}_{FN}, whose ground state is just ψ_G for $r = -1/(1 + \gamma)$. This parameter is then changed in order to be as close as possible to the true hamiltonian for $\gamma \geq 0$, when computations free of sign problem are possible. Indeed in order to improve H^{γ}_{FN} it is very useful to notice that $H^{\gamma}_{FN} = H$, the exact hamiltonian, for $\gamma = -1$ and any non-zero r. Thus at finite positive γ an optimal variational parameter r can be used, that on a lattice, maybe significantly different from the fixed node value $r = 0$, since this value represents the optimal one only in a continuous model, when there exists a rigorous proof that $r = 0$ provides the minimum possible energy.

In order to determine a feasible scheme for the optimization of r in the lattice case, we need to implement small modifications of the Green function (15). We notice that there are two important changes of this Green function that are easily implemented:

4.1 One lanczos step improvement

In this case the Green function (15) is modified by:

$$G^{\gamma}_{1LS} = r_{x'} G^{\gamma}_{x',x} / r_x \tag{19}$$

where $r_x = 1 + \alpha e_L(x)$. After applying statistically the above Green function, after a large number of iterations the configurations x, will be distributed according to the weight (not necessarily positive):

$$\psi_G(x)\psi_1(x)$$

where

$$\psi_1 = (1 + \alpha H)|\psi_G\rangle = \sum_x r_x \psi_G(x)|x\rangle \tag{20}$$

is the first Lanczos step wavefunction as described in Eq. (1). Since the Lanczos iteration improves the wavefunction and the factor r_x has not a definite sign on each configuration

x, it is clear that the phases of the ground state wavefunction are much better represented by the signs of $r_x \psi_G(x)$ rather than by the ones corresponding to $\psi_G(x)$. The parameter $\alpha = \alpha_1/\alpha_0$ can be determined by satisfying the SR conditions[3]:

$$\langle \psi_G | H(\alpha_0 + \alpha_1 e_L) | \psi_n \rangle = \langle \psi_G H(\Lambda - H) | \psi_n \rangle$$
$$\langle \psi_G | (\alpha_0 - \alpha_1 e_L) | \psi_n \rangle = \langle \psi_G | (\Lambda - H) | \psi_n \rangle \tag{21}$$

where $\alpha_i, i = 0, 1$ are computed statistically at any given iteration n in order to improve the SR state $r_x \psi_n(x)$, until convergence is reached for large n. In this case $\psi_n(x)$ is independent of n and statistically equal to ψ_G, whereas α will converge (statistically) to the exact one Lanczos step value. Once this value is determined the energy expectation value over ψ_1 can be evaluated by statistically averaging the local energy $e_L(x)$ corresponding to ψ_G (and not to ψ_1), providing a substantial reduction of computational effort. In this case, since the value of γ is immaterial for the statistical averages, it is more convenient to use $\gamma = 1$, that minimizes statistical fluctuations.

In general, the use of the SR conditions[3] allows to obtain the energy and correlation expectation values of the $p-$Lanczos step wavefunction ψ_p, by using a guiding function ψ_G containing only $p - 1$ powers of the Hamiltonian, e.g. $|\psi_G\rangle \rightarrow |\psi_{p-1}\rangle$. The use of $|\psi_{p-1}\rangle$ as a guiding function for sampling ψ_p may not be the optimal choice. In the following we describe a guiding function with better nodes than ψ_{p-1} but with the same number $p - 1$ of hamiltonian powers, that will be used in the following sections whenever the method SR will be applied,

Using the root decomposition (4) of the $H - polynomial$ defining the $p-$Lanczos step wavefunction $|\psi_p\rangle$, we can single out any real root z_k and similarly to the first Lanczos step case:

$$\psi_p(x) = r_x \psi_G(x) \quad with$$
$$r_x = 1 - e_L(x)/z_k$$
$$|\psi_G\rangle \rightarrow \prod_{i \neq k} (1 - H/z_i) |\psi_G\rangle \tag{22}$$

The new local energy $e_L(x)$, obtained with the new guiding function, will keep into account the phases of the $p-$ Lanczos step wavefunction exactly. In this way, within this decomposition, it is clear that the best guiding function ψ_G of the previous form, is obtained by choosing the real root z_k such that:

$$< 1 - e_L(x)/z_k > \tag{23}$$

is as far as possible (on average over ψ_G) from the zero value. This condition (23) will minimize the sign changes of $\psi_G(x)$ to obtain $\psi_p(x) = (1 - e_L(x)/z_k)\psi_G(x)$, thus providing the best possible phases that we can safely obtain with $p - 1$ powers of the hamiltonian applied to the bare ψ_G.

4.2 Fixed node improvement

In this case the Green function is modified similarly:

$$G'_{FN} = r_{x'} G^\gamma_{x',x} / Sgn(r_x) \tag{24}$$

It is easily obtained that for $r_x = 1 - \frac{1+r(1+\gamma)}{\Lambda} e_L(x)$ and large shift Λ, the effective hamiltonian H_{FN}^γ (8) is indeed considered, as for $\Lambda \to \infty$ the matrix elements of G_{FN} (18) coincide with the ones defined above for $\Lambda G'_{FN}$. up to $O(\frac{1}{\Lambda})$.

In particular for $r = 0$, and $\gamma = 0$ we recover the standard fixed node[8]. Notice also that, if the hamiltonian is free of sign problem $\mathcal{V}_{sf}(x) = 0$ and the fixed node is exact. Then the choice $r = 0$ provides the exact sampling of the ground state of H even for finite Λ, as the factor r_x is proportional to z_x (16) and simplifies in (18,15).

4.3 Generalized Lanczos

Using the above Green function (24), the parameter $r = \frac{-(\Lambda \alpha_1/\alpha_0)-1}{1+\gamma}$, a single parameter at any order p of the Lanczos iterations, is optimized using the SR conditions(21) with ψ_n now depending explicitly on n and differing from the initial guiding function ψ_G: $r_x \psi_n(x) = (G'_{FN})^n \psi_G$. These conditions provide, as mentioned before, α_0, α_1 statistically.[3]: However, in this case, the parameter r, determined by the SR condition, may not coincide with the lowest possible energy condition. A further modification of the Green function[3]

$$G'_\eta = r_{x'} G^\gamma_{x',x}/|r_x|^{1-\eta} Sgn(r_x) \tag{25}$$

that interpolates between the Lanczos limit (19) for $\eta = 0$ (when the SR conditions coincide with the Euler condition of minimum energy) and the fixed node limit (24) for $\eta = 1$ allows to overcome this difficulty, as we get closer but not exactly equal to the Lanczos limit, and one can obtain even lower variational energies.[3]

For the $t - J$ model we avoid to consider here this extra-complication, since the SR conditions (21) have been tested to coincide almost exactly with the Euler conditions of minimum energy (see Fig.2) even for $\eta = 1$ at least for $\Lambda = 0$. As shown in the same figure the SR may also provide a slightly lower energy than the corresponding one obtained by the best r effective hamiltonian H_{FN}^γ, because for small Λ the factor r_x in Eq.(24) may change sign and can correct also the phases of the wavefunction and not only the amplitudes. This is also the reason to work with the minimum possible shift Λ. In principle it is possible to further improve the variational energy and the nodes of the sampled wavefunction, by performing the reconfiguration scheme each k_p steps, with an effective Green function:

$$G'_{k_p} = r_{x'} (G^\gamma)^{k_p}_{x',x}/Sgn(r_x) \tag{26}$$

For $\gamma = 1$, it is possible to work with $k_p > 1$ and with reasonable statistical fluctuations (that increase obviously with k_p). By increasing k_p the factor r_x provides non trivial changes to the phase of the wavefunction with corresponding improvement in energy expectation value. We have not systematically studied this possible modification of the method so far. This extension to $k_p > 1$ should be clearly useful for model hamiltonians, such as the Hubbard model at strong coupling, when a large shift Λ is required for the convergence of the method.

For $\Lambda = 0$ or finite, the coefficient r in the factor r_x may have little to do with the coefficient appearing in H_{FN}^γ, but, even at finite Λ, an effective hamiltonian can be still defined[3], which is qualitatively similar to H_{FN}^γ. In the following discussions we will not consider the difference between the finite Λ effective hamiltonian and the infinite Λ one (8) because it is irrelevant for our purposes.

At each iteration p of the generalized Lanczos the special guiding function described in Eq. (22) is used, yielding optimal phases as close as possible to the $p-$Lanczos step wavefunction. As far as the remaining parameter γ, this is restricted to be positive for statistical reasons (no sign problem). Clearly from property (12), the smaller is γ, the better is the variational energy but increased fluctuations occurs for computing the SR conditions (21). On the other hand, the Green-function shift Λ has to be taken as small as possible, compatibly with $\Lambda - H_{x,x} > 0$ for any x. in order to further improve the efficiency of the power method. Within the SR method by minimizing at best the parameters γ and Λ (or increasing k_p) we can further improve this technique, in a practical scheme. The optimization of the parameter r, since it affects a change in the effective hamiltonian H^γ is particularly important for correlation functions. Instead all the other parameters (including η or k_p for instance) may help to obtain slightly lower variational energies, but are in general much less important. The variational SR results for the $t-J$ model, described in the following sections, are obtained with $\gamma = 1/4$ and $\Lambda = 0$ and refer to the fixed node Green function (24), whereas the symbol FN will always refer to the standard fixed-node case $\Lambda \to \infty$, $\gamma = r = 0$.

5   Results on the t-J model

We consider the pairing correlations in the $t-J$ model for square clusters with periodic boundary conditions:

$$P_{i,j;k,l} = \langle \Delta_{i,j}^\dagger \Delta_{k,l} \rangle$$
$$\Delta_{i,j}^\dagger = c_{i,\uparrow}^\dagger c_{j,\downarrow}^\dagger + \quad i \leftrightarrow j \tag{27}$$

$\Delta_{i,j}^\dagger$ creates a singlet pair in the sites i, j. On each lattice we take the first nearest neighbor pair i, j fixed and move k, l parallel or perpendicular to the direction i, j. In all cases studied the parallel correlations are positive and the perpendicular ones are negative, consistent with a $d-$wave symmetry of the pairing. The existence of phase coherence in the thermodynamic limit is obtained whenever $P_{i,j;k,l}$ remains finite for large distance separation between the pair i, j and k, l. A systematic study has been reported in[17]. Here we focus only on few test cases to show the power of the method, and the importance to work with an effective hamiltonian H_{FN}^γ with a single variational parameter r as described in the previous section. For all cluster used the distance between pair i, j and pair k, l refers to the minimum one between $|R_i - R_k|$, $|R_i - R_l|$, $|R_j - R_k|$ and $|R_j - R_l|$. Only for the $6x6$ we use the so called Manhattan distance $|(x, y)| = |x| + |y|$, since the pair (k, l) in this case is moved in both perpendicular directions. First the pair (k, l) is translated parallel to the x-axis up to the maximum distance allowed by PBC, and then (for the $6x6$) the pair (k, l) is moved parallel to the $y-$ axis.

First of all, whenever the initial variational wavefunction used is qualitatively correct (5), few Lanczos iterations are really enough to obtain exact ground state properties. This is clearly shown in Fig.(3) where the exact results coincide within few error bars with the variance extrapolated results, that in turn are very close to the $p = 2$ Lanczos wavefunction results. However for larger system when the solution is not known, few Lanczos iterations, though systematically improving the energy, cannot change qualitatively the pairing correlations of the initial wavefunction, and in general the variational approach is not reliable.
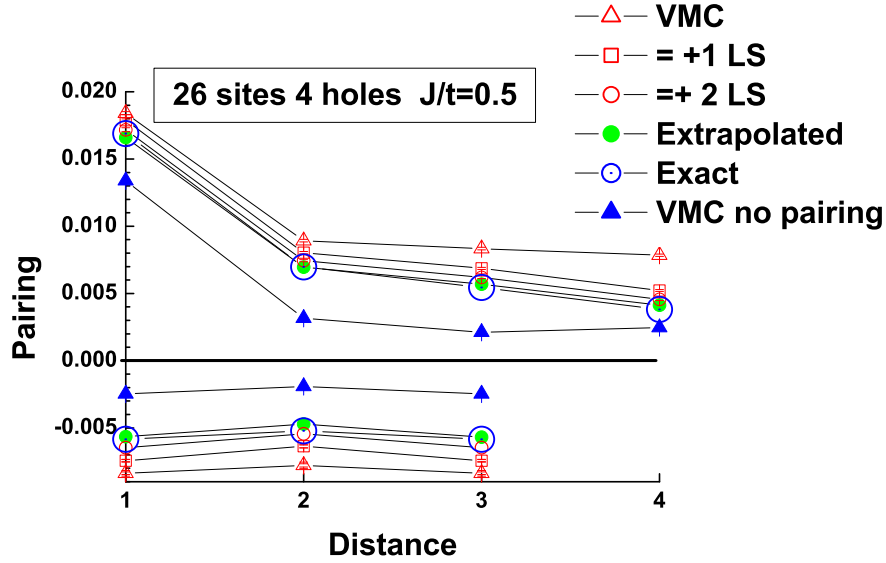
Figure 3. Pairing correlations in the 26 lattice for 4 holes in the $J/t = 0.5\ t-J$ model for the variational Lanczos technique as compared with the exact result obtained with exact diagonalization. The variance extrapolated values are obtained using only the $p = 0, 1, 2$ results available with the statistical algorithm also for much larger system size.

In order to show this effect, we have used two different variational wavefunctions on a 6×6 4-holes $J/t = 0.5$ cluster, and improved both initializations with the methods described in the previous section: the pure variational Lanczos technique, the standard fixed node (FN) and the "generalized Lanczos method" (SR), within the simplified scheme considered before. For one wavefunction initialization, the BCS variational parameters are optimized by minimizing the energy, for the other one we have reduced to a very small value $\simeq 10^{-4}$ the corresponding variational parameter Δ_{BCS} in (6), just in order to remove the degeneracy of the free-electron determinant in the $6x6$. This choice yields a variational wavefunction with definite quantum numbers and with small pairing correlations.

We see in Fig.(4), top panels, that the Lanczos technique is very much dependent on the two different initial choices, even though the energy is in both cases very much improved by few Lanczos iterations. As shown in Fig.(5), the variance extrapolated results of the energy are consistent for both initial wavefunctions. On the other hand the pairing correlations remain inconsistent for about a factor two at large distance.

In this example we clearly see the limitation of the straightforward variational technique: within a very similar energy (e.g. the extrapolated ones) the pairing correlations maybe even qualitatively different.

A completely different behavior is obtained as soon as the FN is applied (middle panels in Fig. 4). The energy improvement within this technique is apparently marginal compared
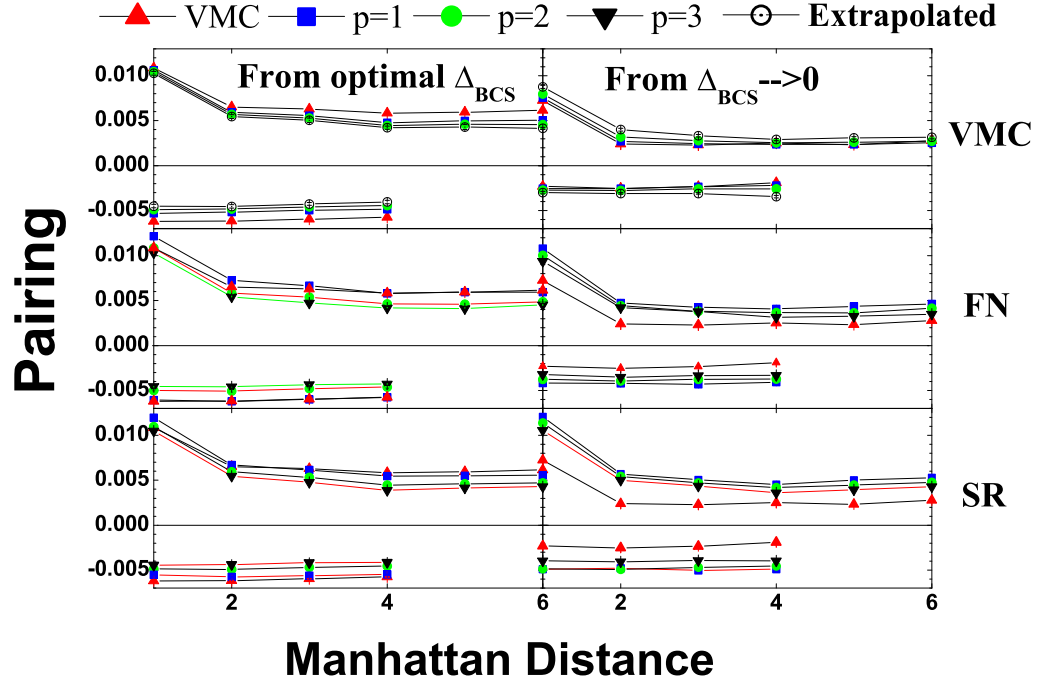
Figure 4. Pairing correlations in the $6x6$ lattice for 4 holes in the $J/t = 0.5\ t - J$ model. Left panels and right panels refer to two different initial guiding functions with or with vanishing small d-wave order parameter respectively. The latter is used in order to remove the degeneracy of the free electron Slater-determinant. The panels at different raws refer to different methods, as a function p of the hamiltonian powers used to evaluate the local energy e_L, required by all the methods: the larger is p, the more (L^p for $p \geq 2$) computationally demanding is the calculation. The VMC values (red trangles) are plotted in all panels for comparison.

to the standard Lanczos technique (see Fig. 5). Instead the behavior of pairing correlations is much better, and already the simple fixed node approximation applied to the pairing correlations is rather independent of the initial wavefunction. The only drawback of this technique is that when systematic improvements to the variational wavefunction are implemented (larger p in the figure), the convergence properties are not behaving so accurately, as one could expect from the convergence of the energy reported in Fig.(5). In particular, even at the most accurate level of this fixed-node approximation -namely the fixed node over the two Lanczos step wavefunction- the two different initializations give pairing correlations differing by about 20% at the largest distance. This is much better than the straightforward Lanczos variational technique (this difference was about 70% for the corresponding two Lanczos step wavefunctions) but is not satisfactory enough.

The reason of such behavior is easily understood in terms of the effective hamiltonian approach. In a lattice case it appears really important for correlation functions to optimize
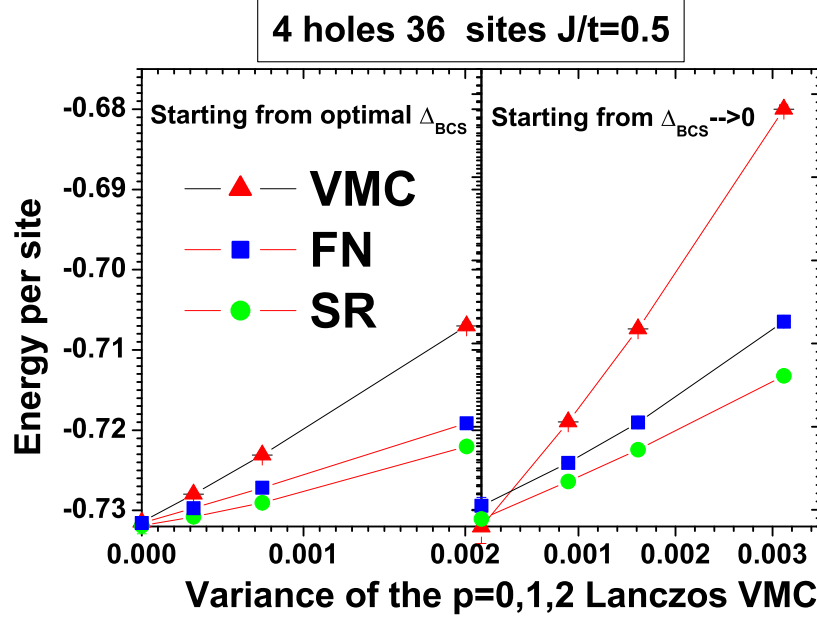
Figure 5. Variational energies obtained with various methods as a function of the variance per site σ^2/L^2 of the p−Lanczos step wavefunction (VMC), which is improved either with standard fixed node (FN) or the generalized Lanczos (SR), with the simplified and efficient scheme described in the previous section. The values at zero variance are extrapolations with a quadratic least square fit.

the parameter r appearing in the effective hamiltonian (8) and not just taking the FN ansatz $r = 0$. This optimization scheme is particularly important whenever some correlations that are not included at the variational level (or much depressed as in the case studied) are increasing as we go down in energy with the help of the improved $p − 1$ ($p > 1$) Lanczos step guiding function. In general for larger p the parameter r increases, thus the SR scheme provides correlation functions substantially different and more accurate than the FN. In the bottom panels it is remarkable that, after applying only 3−steps of the SR technique, both initializations *provide the same results within error bars ($\leq 3\%$) at the largest distance*. These results can be considered benchmark accurate calculations of pairing correlations in the $6x6$ cluster. These pairing correlations clearly indicate a robust d−wave superconducting ground state in the $t − J$ model, at least for this J/t ratio. In this example we notice that correlation functions, in the effective hamiltonian approach, begin to be consistent within 5% whenever the variational energy is accurate within $\sim 1\%$, that is at least one order of magnitude better than a straightforward variational technique like the Lanczos one.

Of course for larger size, consistent correlation functions, i.e. independent from the initial wavefunction with or without Δ_{BCS}, can be obtained for a larger number p of SR-
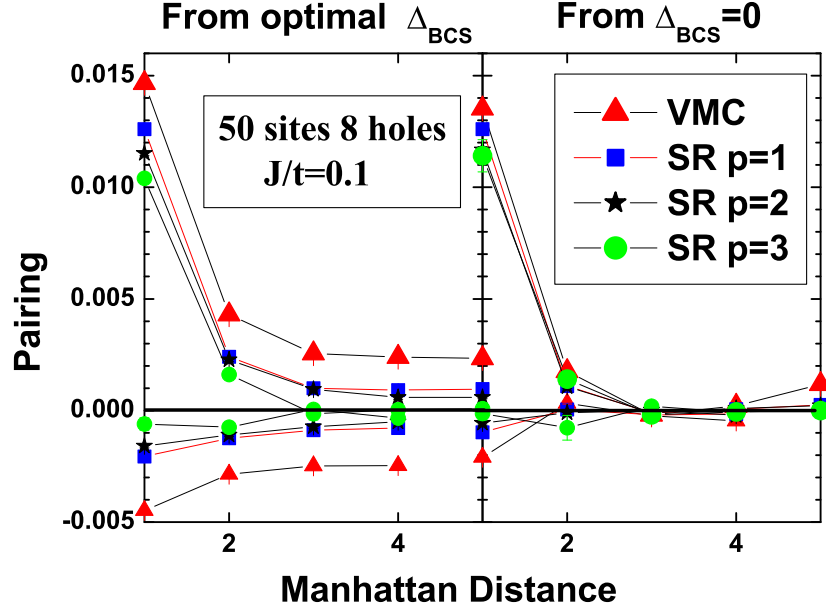
Figure 6. Pairing correlations in the 50 site lattice for 8 holes in the $J/t = 0.1$ $t - J$ model. Left panels and right panels refers to different initial guiding function with or without d-wave order parameter respectively. The pairing correlations for both calculations are consistently small at the most accurate level of approximation (SR $p = 3$).

iterations. Here we report a sample case for a 50 site cluster at small $J/t = 0.1$. We see in Fig.(6) that the sizable pairing correlations present in the variational wavefunction with $\Delta_{BCS} \neq 0$, represents just an artifact of the variational calculation. At the third step, of the SR technique, when, as shown in Fig.(7) we reach an accuracy in energy below 1% (assuming that the variance extrapolated energies-both consistent- are exact), the pairing correlations are again consistent within few error bars, and clearly vanishingly small at large distance.

6   Conclusions

We have shown that within a brute force variational technique, such as the Lanczos method for few iterations, it is hard to obtain accurate values of correlation functions unless the energy accuracy is far from the present possibilities, at least in two dimensions. An accuracy of about one part over 10^4 in the energy would be probably possible with at least 10 Lanczos steps or 100000 states in DMRG 2D calculations for systems of about 100 sites with periodic boundary conditions. This kind of accuracy maybe enough to obtain consistent correlation functions even within these two variational methods, but is far from being
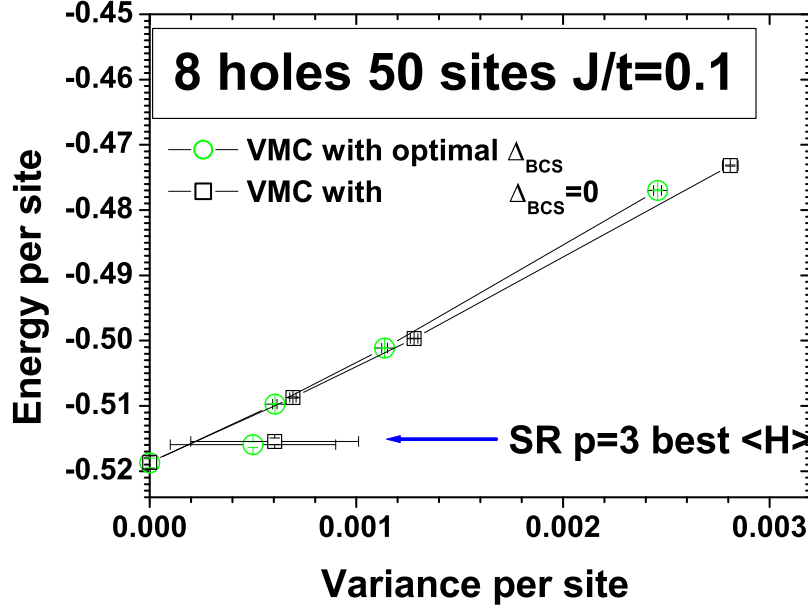
Figure 7. Variational energy as a function of the variance per site σ^2/L^2 for the $p-$Lanczos step wavefunction (VMC), which is improved by the "generalized Lanczos method" (SR). The best variational SR $p = 3$ energies are indicated by the arrows.

possible at present.

We have shown instead that a qualitatively different and very promising approach, based on the optimization of an effective hamiltonian, rather than adding more variational parameters in a brute force variational scheme, appears to be very useful to control correlation functions. The idea is based on the "effective hamiltonian approach" described in the introduction.In this scheme it is assumed that between similar Hamiltonians, the correlation functions of their ground states should be also similar. The SR technique, allows to systematically improve the effective hamiltonian considered even compared to the lattice fixed node one[8], with an iterative scheme very similar to the Lanczos one, thus the name "generalized Lanczos".

Within this scheme it is clear that there are robust pairing correlations in the $t - J$ model at sizable but not unphysical value of J/t[17]. However there exists a critical value $(J/t)_c \geq 0.1$ below which pairing correlations are clearly suppressed. The existence of such a critical $(J/t)_c$ is clearly understood because at $J/t = 0$, the ferromagnetic instability takes place even at large doping [18].

Acknowledgments

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